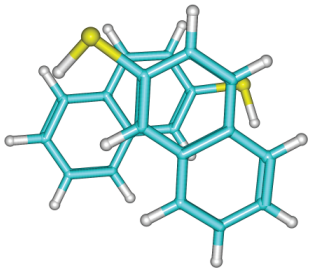
OBSERVATION OF 2-NAPHTHALENETHIOL HOMODIMER USING ROTATIONAL SPECTROSCOPY

RIZALINA TAMA SARAGI, MARCOS JUANES, ALBERTO LESARRI, *Departamento de Química Física y Química Inorgánica, Universidad de Valladolid, Valladolid, Spain*; LOURDES ENRIQUEZ, MARTIN JARAIZ, *Departamento de Electrónica, ETSIT, University of Valladolid, Valladolid, SPAIN*.

Following previous studies of gas-phase dimerization of sulfur-bearing aromatic thiols, like thiophenol[a], benzyl mercaptan[b] and 2-phenylethyl mercaptan[c], we conducted a structural investigation of 2-naphthalenethiol using chirped-pulse Fourier transform microwave spectroscopy in a jet-cooled expansion. Two conformers of the monomer have been observed in the frequency region 2-8 GHz. All monosubstituted (^{34}S and ^{13}C) isotopologues could also be observed. Finally, a single isomer of the homodimer of 2-naphthalenethiol was identified. The homodimer is stabilized by π-stacking interactions, with no hydrogen bond interaction between the two thiol groups. Supporting ab initio and DFT calculations will be presented.



[a] R.T. Saragi, M. Juanes, C. Pérez, P. Pinacho, D.P. Tikhonov, W. Caminati, M. Schnell, A. Lesarri, *J. Phys. Chem. Lett.* 2021, 12, 5, 1367–1373.
[b] R.T. Saragi, et al., *in publication* 2021.
[c] R.T. Saragi, et al., *in publication* 2021.